

#### IV. THEORETICAL CALCULATIONS OF THE EXPLOSION

##### A. GENERAL INFORMATION

An explosion is an effect produced by the sudden expansion of gases. If the amount of fuel and air is in proper proportion then a large amount of heat is released (with a corresponding rapid pressure increase) which causes a rapid expansion of the gases. Solid fuels normally burn slowly because fire occurs in the gas phase (the exception being just a very few solids) and the solid must vaporize to release gases which can then diffuse away from the solid to mix with air to burn. This same mechanism for fire occurs with liquid fuel pools or droplets; the liquid must vaporize and diffuse to meet the oxygen in air before it can chemically react in fire. If a gaseous fuel is already mixed with air (called premixed combustion as opposed to diffusion burning), then the time for melting, vaporizing and mixing with air is avoided. In this case, the reaction can occur very rapidly, thereby quickly releasing heat which expands the gases explosively. When these moving gases at high pressure contact an object, the mass-flow with increased pressure can move the object — such as a person being hit by a blast wave.

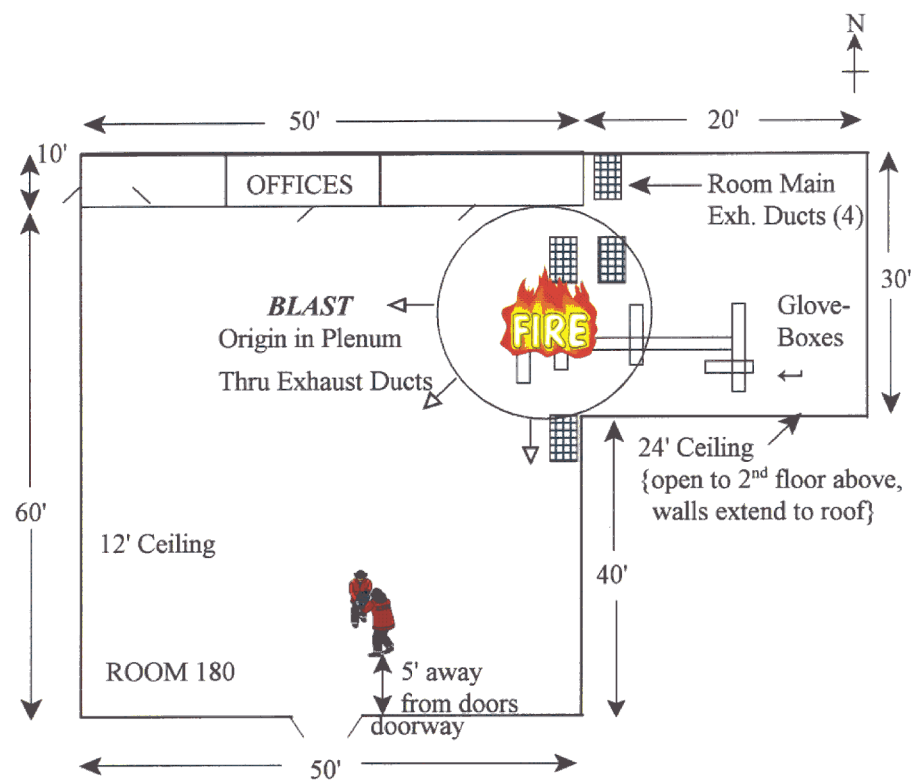
In the event in Room 180, personnel were moved/knocked down by the pressure and corresponding mass-flow impact force on the body. It takes approximately a 1-psi (pounds-per-square-inch) overpressure (i.e., pressure above normal atmospheric pressure of 14.7-psi) to move a person.<sup>(25a)</sup> It will be shown in these calculations that the only plausible event that produced this pressure front was the explosive chemical reaction of very reactive gases produced from thermal degradation and smoldering of the filter media and accumulated lint/dust in the plenum. Lint and its related dust will be referred in this section as “lint.” Heat and burning embers from the fire burning in Room 180 were being exhausted by the building’s Main Exhaust fans immediately downstream of the Plenum to cause heating/ignition of the solid filter media, and accumulated lint on the face of the filters in the Plenum. This heating/ignition caused the filter(s) and lint to release vapors which then reached a critical concentration in mixture with air, and a sudden expansion of the gases in the Plenum occurred. This explosion scenario is described in Section III, subsection B.5a.

Fuel by itself cannot burn, just as air by itself cannot burn. There must be

a proper proportion of fuel and air mixed together, and this proportion has a range such as 25% fuel-in-air to 75% fuel-in-air (these limits for burning possibility are called the lower and upper flammability limits). Therefore, when enough carbon monoxide (CO) and unburned hydrocarbons (UHC) accumulate and mix with air within proper proportions, the rapid chemical reaction in the gas phase then causes a local volume of high temperature and pressure to occur. At this time, it then pushes the surrounding gas outward along available unrestricted flow paths — in this case, the 17 Main Exhaust ducts leading into and the four exhaust fan ducts exiting the Plenum. The outward flow of air and gases from the Plenum, down duct #86 (which the exhaust ducts within Room 180 are tied into) and into Room 180 will be addressed in these calculations.

The explosion calculations that follow will show the amount of filter media and lint needed to produce the size of the explosion required to generate the following inferred overpressures: (a) In Room 180: 1 psig to knock a person down but not above 2 psig since this pressure would have caused eardrum damage and no physical injury was reported<sup>(26a)</sup> (see Figure 1); and (b) in the Plenum and main exhaust ductwork leading to Rm 180: less than 3 psig, since there was no reported structural damage<sup>(26a, 27c)</sup> (see Figure 2).

**Fig. 1. CONFIGURATION OF ROOM 180 AT THE TIME OF THE EXPLOSION**



**Fig. 2. CONFIGURATION OF MAIN EXHAUST SYSTEM DUCTWORK AT PLENUM**

The cross-sectional areas (normal to the axis of airflow) of all 17 Main Exhaust Ducts that enter the north wall of the Plenum are shown in the following schematic.

Note: Numbers in boxes are as follows: # = Duct No. - Duct Opening in square feet):

**Building 71**  
**Plan View of Filter Plenum Area**  
**(No Scale - dim. approx.)**

**B. THERMO-CHEMISTRY OF THE EXPLOSION**

Each of the filters in the Plenum filter bank is 24"W x 24"H x 11.5"D. Clean filters weigh 32 pounds, of which 20 pounds consists of the filter media and 12 pounds is the wood frame. The filter media is primarily cellulose (86%, the remaining 14% is asbestos). This 86% equates to approximately 17.2 pounds of cellulose per clean filter. Dirt on/in the filters is mainly lint which is also cellulose. In addition, cellulose is the chief component of wood and plant fiber; cotton, which lint is comprised of, for instance, is nearly pure cellulose.<sup>(25c)</sup> The chemical formula of cellulose is  $(C_6H_{10}O_5)_n$ . Physical methods give molecular weights for cellulose ranging from 250,000 to 1,000,000 or more. X-ray analysis and electron microscopy indicate that these long chains lie side-by-side in bundles, undoubtedly held together by hydrogen bonds between the numerous neighboring -OH groups. These bundles are twisted together to form rope-like structures, which themselves are grouped to form the fibers we can see." The formula weight for cellulose is 162.14.<sup>(32)</sup>

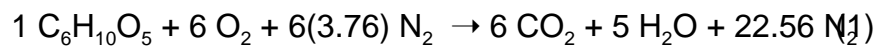
**1. Burning of Cellulose**

The heat of combustion of cellulose is 17.47 MJ/kg<sup>(26b)</sup>. Converting Metric to English units:

$$17.47 \text{ MJ/kg} \times 10^6 \text{ J/MJ} \times \text{Btu}/1055 \text{ J} \times \text{kg}/2.2046 \text{ lbs} = 7511 \text{ Btu/lb.}$$

Air is composed of, approximately, 21% O<sub>2</sub> and 79% N<sub>2</sub> by volume or 1-mole O<sub>2</sub> and 3.76-moles N<sub>2</sub> (79/21 = 3.76).

Complete combustion of cellulose means that all the fuel is converted to carbon dioxide and water, implying that there is sufficient air available to do so. Therefore, the overall chemical reaction (as differentiated from elementary reactions for chemical kinetics) is:



The combustion reaction thermodynamics is

$$Q + \sum n_i h_i = \sum n_e h_e \quad (2)$$

where “Q” is the heat of reaction, “n” is the number of moles of a substance and “h” is the enthalpy of a substance with “i” indicating initial reactants and “e” indicating final products exiting.

Generating the numbers for the reaction (1), using the enthalpy of formation  $h_f$  (noting that  $h_f$  is zero for elements like O<sub>2</sub> and N<sub>2</sub>):

$$\sum n_i h_i = h_f^{\text{cell}} \text{ (of cellulose)} + 6 (0) + 6(3.76)(0) = h_f \text{ of cellulose}$$

$$\sum n_e h_e = 6 h_f^{\text{CO}_2} + 5 h_f^{\text{H}_2\text{O}} + 22.56 (0) = 6 (-169,297) + 5(-104,036)$$

$$= -1,535,962 \text{ Btu/lbmol}$$

Using equation (2) and noting that heat given off is negative:

$$Q = -1,535,962 - h_f^{\text{cell}} = -7511 \text{ Btu/lb} \times 162.14 \text{ lb/lbmol} = -1,217,568.76 \text{ Btu/lbmol}$$

since the molecular weight is the number of pounds (lb) in a pound-mole (lbmol).

Rearranging the above, the heat of formation of cellulose is obtained:

$$h_f^{\text{cell}} = -1,535,962 + 2,217,568.76 = -318,393 \text{ Btu/lbmol. (3)}$$

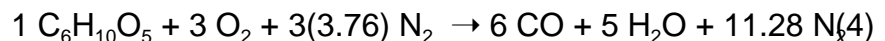
This value is needed for calculations in sub-section B.2. which follows.

## 2. Smoldering of Cellulose

Smoldering combustion is self-sustaining whereas pyrolysis requires an external heat source. While most materials can be pyrolyzed, only a few materials, including cellulosic materials, are able to smolder. Pyrolysis and smoldering occur at a fuel surface as a result of elevated temperature, and the temperature of a pyrolyzing sample (600 to 900 Kelvin) is much less than the gas phase flame temperature (1200 to 1700 Kelvin).

“The decomposition of cellulose involves at least four processes in addition to simple desorption of physically bound water.”<sup>(27)</sup> The first is dehydration, second is the unzipping of the cellulose chain, third is the decomposition of the dehydrated product (dehydrocellulose), and finally “to decompose to yield smaller volatile products, including CO.”

The smoldering of cellulose is denoted by the following overall chemical reaction:



Note that this is similar to reaction (1) but now there is insufficient oxygen to completely form  $\text{CO}_2$  and instead CO is formed. In actuality, some unburned hydrocarbons would likely form according to the chemical kinetic chain reaction. Hydrocarbon fuels generally react via a set of complex simultaneous, interdependent reactions (chain reactions). A simple set of occurrences representing the detailed elementary chemical reactions of gas phase hydrocarbon fuel burning are summarized as:

- a. The hydrocarbon fuel molecule is broken by (1) collision of an energetic (hot) particle or (2) attack by a flame radical, the latter being an unstable reactive species with an unpaired electron formed by flame reaction, such as O, H and OH.

- b. The radical pool (O+H+OH+others) attacks intermediate species to form a chain reaction from endothermic energy absorbing reactions to exothermic energy releasing reactions.
- c. Hydrogen is stripped from the fuel and intermediate fuel fragments, and oxygen is added. Carbon monoxide is formed by adding oxygen to the hydrogen-stripped carbon fuel.
- d. Finally hydrogen is oxygenated to water and carbon monoxide is oxygenated to carbon dioxide when sufficient air is available by transport processes.
- e. Schematically:  
 $\text{CH}_4 + \text{M}, \text{H}, \text{O}, \text{OH} \text{ (M=any particle)} \rightarrow \text{CH}_x\text{O}_y \text{ (CH}_3, \text{CH}_2\text{O, HCO)}$   
 $\text{CH}_x\text{O}_y + \text{radical pool} \rightarrow \text{CO}$   
 $\text{CO} + \text{O}, \text{OH} \rightarrow \text{CO}_2 \text{ and}$   
 $\text{H}, \text{OH}, \text{M} + \text{O}, \text{O}_2 \rightarrow \text{H}_2 + \text{H}_2\text{O} + \text{M}.$

Using the equation (2) process for equation (4):

$$\begin{aligned}
 Q &= \sum n_e h_e - \sum n_i h_i \\
 &= [6(-47,551) + 5(-104,036) + 0] - [1(-318,393.24) + 3(0) + 11.28(0)] \\
 &= -487,092,76 \text{ Btu/lbmol} \times \text{lbmol}/162.14 \text{ lb} = -3,004.89
 \end{aligned}$$

From equation (4) it is noted that 1 lbmol of the cellulose fuel yields 6 lbmol of CO. Using molecular weights for converting from lbmol to lb:

$$1 \text{ lbmol of cellulose} \times 162.14 \text{ lb/lbmol} \rightarrow 6 \text{ lbmol of CO} \times 28$$

$$\text{or } 162.14 \text{ lb of cellulose fuel} \rightarrow 168 \text{ lb of CO,}$$

that is, about 1 pound of fuel (filter media/lint dust) gives about 1 pound of CO ( $1 \text{ lb}_{\text{cell}} \rightarrow 1 \text{ lb}_{\text{CO}}$ ) within a 3.5% accuracy.

### 3. Amount of CO Needed to Cause Overpressure Within the Plenum

Using the approximation of a “perfect gas,” how much CO would have to be released from the filters and lint, and reacted to produce an estimated 10-psig (“ballpark” range) in the Plenum?

The ideal gas law, which is applicable to gases such as air and CO at pressures below approximately 100-psi, is

$$PV = NRT \quad \text{or} \quad PV/NRT = 1 \quad (5)$$

where P is pressure, V is volume, N is the number of moles, R is the universal gas constant, and T is temperature.

In the volume of the Plenum, the initial conditions related to the final conditions are

$$(PV/NRT)_i = (PV/NRT)_f \quad (6)$$

Since V is the volume of the Plenum, which remains unchanged as the carbon monoxide chemically reacts, then the constant V can be removed from equation (6) by dividing both sides of equation (6) by V. Similarly, R is constant and can be removed from equation (6) by multiplying both sides of equation (6) by R.

Now equation (6) for the Plenum becomes

$$(P/NT)_i = (P/NT)_f \quad \text{or}$$

$$P_i / N_i T_i = P_f / N_f T_f$$

Rearranging the above equation results in:

$$P_f = P_i N_f T_f / N_i T_i \quad (7)$$

To get the initial and final moles (N) for use in equation (7), consider the reaction of carbon monoxide with air in the Plenum:





The initial reactants of carbon monoxide and air on the left side of equation (8) have a total of 3.38 moles ( $1 + \frac{1}{2} + 1.88$ ) and the chemical reaction products have a total of 2.88 moles ( $1 + 1.88$ ).

As an example, for 10-psig overpressure, then  $P_f$  would be  $14.7 + 10 = 24.7$  psia.

If the initial conditions in the Plenum were at standard thermodynamic conditions of 77°F and 14.7-psia, then according to equation (7)

Note: The effect of initial conditions will be shown below to be negligibly small.

$$P_f = (14.7 \times 2.88 \times T_f) / (3.38 \times 537) = 24.7 \text{ psia}$$

where  $P$  has units of psia and  $T$  has units of degrees Rankine ( $^{\circ}\text{R} = ^{\circ}\text{F} + 460$ ).

Solving the last equation for  $T_f$  gives  $T_f = 1059^{\circ}\text{R} = 599^{\circ}\text{F}$ .

Assuming the amount of CO and CO<sub>2</sub> in the air in the Plenum is relatively small (as will be shown below), then the properties of just air can be used to evaluate how much CO would be needed to react in the Plenum to achieve 10-psig overpressure. The internal energy change in the Plenum will now be calculated using tabulated values for air.<sup>(25d)</sup>

The internal energy ( $u$ ) of air at 537 °R is 91.53 Btu/lb and at 1059 °R is 183.29 Btu/lb. Therefore, the change in internal energy of the air in the Plenum is

$$\Delta u = 183.29 - 91.53 = 91.76 \text{ Btu/lb}_{\text{air}} \quad (9)$$

The Plenum is 230' wide x 14'-8" high x 20' deep (minus the volume of the cross-beams = 12 beams x 1' x 2.67' x 20'). Therefore, the total volume of the Plenum is

$$V_{\text{plenum}} = 230' \times 14'-667" \times 20' - 640' = 66,827 \text{ cubic feet}$$

The weight of air at standard thermodynamic conditions is 0.07647

pounds per cubic foot (lb/ft<sup>3</sup>)

Based on the above, the amount of air in the Plenum that received the internal energy change in equation (9) is

$$66,827 \text{ ft}^3 \times 0.07647 \text{ lb/ft}^3 = 5,110 \text{ lb}_{\text{air}}$$

Therefore, to cause the internal energy change needed for 10-psig overpressure according to equation (9) requires an energy input to the air in the Plenum of

$$91.76 \text{ Btu/lb}_{\text{air}} \times 5,110 \text{ lb}_{\text{air}} = 468,893.6 \text{ Btu}$$

The value for the heat of reaction of CO is 10.10 MJ/kg<sup>(26b)</sup> which in English units is

$$(10.10 \text{ MJ/kg}) \times (10^6 \text{ J/MJ}) \times (\text{Btu}/1.055 \times 10^3 \text{ J}) \times (\text{kg}/2.2046 \text{ lb}) \\ = 4,342 \text{ Btu/lb}_{\text{CO}}$$

Therefore, the number of pounds of CO that are needed to react to put 452,836 Btu into the air in the Plenum is

$$468,893.6 \text{ Btu} / 4,342 \text{ Btu/lb}_{\text{CO}} = 108 \text{ lb}_{\text{CO}}$$

Note: 108 pounds of CO is about 2% relative to 5,110 pounds of air in the Plenum; therefore, the use of internal energies for air alone is validated.

In subsection 2. above, it was shown that one pound of fuel (cellulose filter media) yields approximately one pound of CO within 3.5% accuracy. Since one filter has approximately 17.2 pounds of cellulose, then to get 108 pounds of CO requires approximately 108 pounds of filter media. This equates to approximately 6.3 clean or 4.6 dirty filters (each with six pounds of lint/dust), or approximately 19 clean or 14 dirty filters burned one-third of the way which can react to cause a 10-psi overpressure in the Plenum.

Changing the temperature in the Plenum to 300°F (temperature at which the filter media adhesive and rubber gaskets fail), instead of 77°F as calculated above, then according to equation (7)

$$P_f = (14.7 \times 2.88 \times T_f) / (3.38 \times 760) = 24.7 \text{ psia}$$

where 537 used previously was replaced with 760.

Solving for  $T_f$  gives 1499 °R as compared to the previous value of 1059 °R as calculated above using 537 °R. Using equation (9) again, but with the different values for internal energy gives

$$\Delta u = 266.34 - 91.53 = 174.81 \text{ Btu/lb}_{\text{air}}$$

$$174.81 \text{ Btu/lb}_{\text{air}} \times 5,110 \text{ lb}_{\text{air}} = 893,279.1 \text{ Btu}$$

$$893,279.1 \text{ Btu} / 4,342 \text{ Btu/lb}_{\text{CO}} = 205.7 \text{ lb}_{\text{CO}}$$

therefore, to get 205.7 lb<sub>CO</sub> requires about 205.7 lb of filter media or approximately 12 clean or 9 dirty filters.

The calculations above were exemplary and were for 10-psig overpressure “ballpark” range in the entire Plenum. They were performed to indicate the correctness of the postulation that a reasonable amount (according to “after-the-fact” analysis) of filters in the Plenum could yield enough reactive gas to cause an explosion that was of the “order of magnitude” indicated by this analysis. However, the actual overpressure, at the time of the explosion during the 1957 fire, could not have been a ten psig overpressure! The actual resultant damage based on information contained in, and assumptions made from, the Original Rocky Flats Fire Report and associated photographs, appears to indicate that the overpressure in the Plenum did not even exceed three psig.<sup>(26a)</sup>

Note: Table 4-2B in the cited reference shows overpressures of 2-3 psi would result in shattering of 12" thick unreinforced concrete wall panel. While the plenum walls were 12" reinforced walls, no structural damage of any type was reported.

The amount of CO required to achieve the lower stated overpressure of less than three psig, within the plenum at the time of the explosion in 1957, will be shown in the following subsection.

### C. POSTULATIONS FOR THE PLENUM EXPLOSION

It was shown in subsection IV.B. above that the reasonableness of the postulated scenario for filter media smoldering is validated. That is, the amount of filter media needed for the “ballpark” range of 10 psi overpressure and temperature are reasonable with respect to the observed filter damage (via original Rocky Flats Fire Report after-fire photographs) in the Plenum. These results are in agreement with previously conducted Filter Fire Tests addressed in Section III.B. of this Report. These tests showed that the filters ignite at 419°F and that the adhesives melt and rubber gaskets fail at about 300°F. Therefore, the temperature of 300°F previously calculated is a reasonable temperature for the flow of hot gases into the Plenum from ductwork #86, which is connected to exhaust ductwork in Room 180. The 300°F is considered a reasonable temperature for the hot gases entering the Plenum and is a much different temperature from the burning process of cellulose. Smoldering is an actual burning process, although it is quite different from flaming. Temperatures in the smolder zone are typically 900-1600°F, whereas the temperatures reached in a flame are much higher.

It is postulated that the flow of hot gases and burning embers due to the fire in Room 180, into duct #86, were the cause of heating and ignition of the filter media. The resultant heating and ignition of filter media in the Plenum would be at an area downstream of exhaust duct #86 in the “dirty air” side of the Plenum. The description “downstream” is used to denote the hot airflow pattern as determined by the duct, plenum and main exhaust fan configurations. That is, as the hot air flows from duct #86 into the Plenum it may not flow in a geometric direction directly across from the connection of duct #86 to the Plenum because of the airflow patterns. However, relatively-heavy burning embers may not directly follow the airflow path because of inertia.

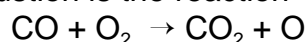
The heating of the filter media and lint in the Plenum, due to the hot gases and possibly burning embers and/or sparks from the fire in Room 180 caused smoldering of the cellulosic filter media and lint/dust in the plenum. It is postulated that, according to hydrocarbon chemistry, the result of heating the filter media and lint produced the formation of carbon monoxide (CO) and unburned hydrocarbons (UHC) in the inlet (“dirty air”:) side of the Plenum. The CO and UHC formed a concentration that became flammable and explosive in air, which is in agreement with the results obtained in the Filter Fire Tests; i.e., ignition of the filters and a “flame flashback” or minor

explosion.

Exemplary calculations presented in the previous Subsection IV.B. show that CO released from an estimated number of filters can combust and yield an energy release to cause the “ballpark” range of 10 psi overpressure in the Plenum. The use of CO alone and not UHC in the calculations is validated by the facts that (a) past filter fire tests, referenced in Section III of this Report, show that a “minor explosion” occurs in burning filters and (b) the heat of combustion per mass of air consumed is nearly constant for most organic fuels;<sup>(25e)</sup> the NFPA Fire Protection Handbook states “It can be shown that a value of  $\Delta h_f/r = 3.0\text{MJ/kg air}$  is near-constant. An assumption of constant heat of combustion per kilogram of air is useful in heat release rate measurements and for air-limited combustion problems.”<sup>(26b)</sup>

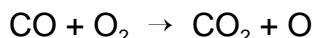
The reaction of carbon monoxide with the oxygen in air can be explosively fast and information will now be provided about the chemical reaction kinetics of carbon monoxide. It is important to differentiate between “dry” and “wet” carbon monoxide oxidation. It is known that as little as 20 ppm (0.2% = 0.002) of water can completely change the reaction of CO, with “dry-CO” oxidation being slower than “wet-CO” oxidation, and it is known that water was used to extinguish the fire in Room 180 just a minute or two before the explosion. The following quotes are from the book entitled “Combustion.”<sup>(25e)</sup>

“It is very important to note that the presence of any hydrogen containing material can completely alter the picture and, in fact, there is agreement in the oxidation of “wet” carbon monoxide. Only 20 ppm of hydrogen can change the complete mechanism of carbon monoxide; thus in most practical systems, carbon monoxide will proceed through this so-called “wet” route .... It is therefore seen that the low pressure ignition of CO-O<sub>2</sub> is characterized by an explosion peninsula, just as in the case of H<sub>2</sub>-O<sub>2</sub> .... It is generally agreed that the most likely chain initiating step in the dry combustion is the reaction

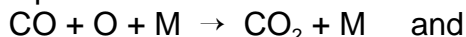


which is exothermic and should proceed readily .... Brokaw offers the speculation that explosions in this system are thermally initiated by the nearly thermo-

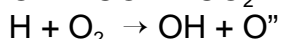
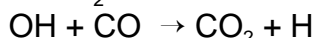
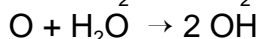
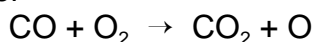
neutral reaction



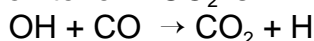
with subsequent large energy release through the third-body steps



“Very early, from the analysis of ignition, flame spread, and detonation velocity data, investigators realized that small concentrations of hydrogen-containing material would appreciably catalyze the kinetics of CO-O<sub>2</sub>. The H<sub>2</sub>O catalyzed reaction proceeds in the following manner



“It is generally agreed that the important step in wet CO oxidation to form CO<sub>2</sub> is



This reaction is known to be quite rapid and important in later stages of hydrocarbon oxidation .... As would be expected, the presence of water broadens the explosion peninsula and extends it to lower temperatures.”

The above statements, therefore, support the postulate that the heating of the filter media resulted in an explosive “wet” CO reaction.

An explosive medium may support either a deflagration or detonation wave depending upon various conditions, the most obvious being confinement and mixture ratio. The primary result of an ordinary thermal initiation appears always to be a flame which propagates at subsonic speed. Where conditions are such that the flame causes adiabatic compression of the still unreacted material ahead of it, the flame velocity speeds up. In some observations, the speed of the flame seems gradually to rise until it equals that of a detonation wave. An explosion may result from chemical changes such as the combustion of a flammable gas-air mixture. Associated with the term explosion are the terms “deflagration” and “detonation”. A deflagration is an exothermic reaction which propagates from the burning gases to the

unreacted material by conduction, convection, and radiation. In this process the combustion zone progresses through the material at a rate that is less than the speed of sound in the unreacted materials. In contrast, a detonation is an exothermic reaction characterized by the presence of a shock wave in the material which establishes and maintains the reaction. A distinctive difference is that the reaction zone in a detonation propagates at a rate greater than the speed of sound in the unreacted material. The principal heating mechanism is one of shock compression; the temperature rise is directly associated with the intensity of the shock wave, rather than being determined by thermal conductivity. A shock wave will cause initiation of a detonation directly, whereas lower intensity ignition sources (e.g., burning embers) will not. Due to the presence of the 17 exhaust ducts entering the plenum's upstream ("dirty air") side and four exhaust fan ducts discharging from the downstream ("clean air") side, "total containment" did not exist within the Plenum. Since a very large ignition source is needed for a detonation (which did not exist in the Plenum), it can be safely stated that the explosion in the Plenum was a deflagration. The term "Vapor Cloud Explosion" has been used to describe the effects of igniting a large unconfined vapor cloud whereby significant overpressures are generated. Maximum pressures of approximately eight times the initial pressure can result from deflagrations of stoichiometric gas-air mixtures. The adiabatic flame temperature for stoichiometric combustion of CO was calculated and used to generate a maximum explosion pressure of 94-psi in 300°F (149°C) air; therefore, the explosion in the Plenum was a "minor explosion" (a few psi). A vapor cloud explosion or decomposition explosion, due to the decomposition products from the smoldering of cellulose (both the filter media and suspended lint/dust) with a resultant deflagration ignited by various occurring flame flashbacks, is what is postulated to have occurred in the Plenum (see Figure 3).

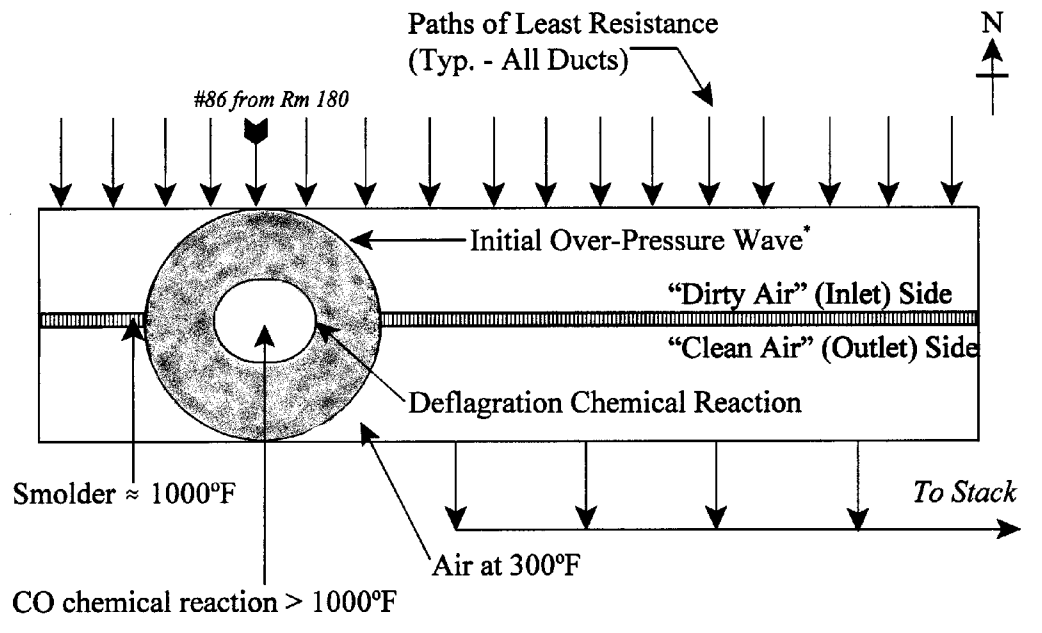
In summary of the heating events, the fire in Room 180 caused the air in the room and the air that is exhausting to the plenum to be heated. Since the filter adhesives are not believed to have catastrophically failed, then it is assumed that the overall air in the plenum could have been around 300°F (149°C). The smoldering within the cellulosic filter media and lint/dust to generate CO could have been above 1000°F (538°C). However, when the kinetic chemical reaction of CO occurs, then the temperature local to the filter media would increase due to the chemical heat release. The rapid expansion of the gas near the filter media aided in intensity by the lint/dust generated into suspension by the "flame flashbacks" was caused by the

rapid chemical reaction of CO, which then caused the corresponding rapid increase in local temperature. This rapid expansion of gas is the initial vapor cloud explosion. This expansion (explosion) of gas then generated a gas dynamic wave (i.e., the blast wave) with attendant overpressure that traveled into the 300°F (149°C) air and through the ducts. This is illustrated in the depiction of the pressure wave in the plenum shown in Figure 3.

If a deflagration proceeds at a speed less than the speed of sound, and gas dynamics theory shows that a pressure increase can only occur with a shock wave traveling greater than the speed of sound, then how is this reconciled? This is an often misunderstood situation and an often encountered dichotomy. Human speech generates sound waves that travel from the mouth at the speed of sound, i.e., sonic speed, and this is not a very intense source of generation! What is needed here is a proper understanding of the locations of the waves. When one refers to a deflagration, one is referring to the speed of the flame front into the unburned flammable gas-air mixture. The speed of this flame front or wave is indicative of the speed of the chemical reaction and heat transfer. This deflagration flame speed is not the speed of the pressure pulse transmitted beyond the flammable gas-air mixture into the surrounding air. The speed of the pressure pulse or wave transmitted into the surrounding air must be supersonic in order to yield a pressure increase. When a small pressure pulse is generated (e.g., by speech or energy release from chemical reaction), the temperature behind the small pressure pulse is slightly higher than in front of the wave. Therefore, the sonic speed ( $\propto \sqrt{T}$ ) behind the small initial pressure pulse is slightly higher than in front, so that another sonic wave traveling behind the first pulse will overtake the first wave and combine with it to increase the pressure of the first wave. Additional pressure pulses catch up with the first wave to overtake and combine with it, and in this manner a shock wave is formed with its attendant pressure increase. Therefore, the situation for a vapor cloud explosion in the Plenum is the rapid: (1) heating in the flammable vapor cloud due to chemical reaction; (2) expansion of the hot gas products in the cloud volume; (3) generation of pressure waves into the air around the burned cloud; (4) formation of a pressure wave with overpressure; and (5) proagation of the overpressure outwardly.

The postulated pressure wave configuration is depicted as follows:





**Fig. 3. POSTULATED PRESSURE (SHOCK) WAVE CONFIGURATION**

\*This "overpressure wave" occurs simultaneously on both sides of the filter bank due to the: (a) porosity of the filter media; (b) numerous openings in the filter bank in this area due to some possibly ruptured filters and burned-through filters; and (c) concentration of smoke on both the inlet and outlet sides of the filters all as described in subsection III.B.5. of the Report.

In effect, the deflagration results in the rapid generation of a hot gas volume that expands and acts like a piston pushing outwardly on the surrounding air. This rushing air pulse (shock wave) with overpressure in turn then goes rushing down all 17 unrestricted ducts connected to the Plenum and into the rooms where these ducts originate. This condition resulted in the: (1) knocking down of personnel in Room 180 and in the adjacent corridor; and (2) gross contamination throughout Building 71. To a lesser degree, some of the air pulse enters into the "clean air" side of the plenum and exhaust ductwork.

# 1. Gas Dynamics<sup>(25f)</sup>

The following data are tabulated values for normal shock waves in air for various overpressures:

Table 1. Normal Shock Values for a Moving Coordinate System from Tables<sup>(25f)</sup>

Overpressure	$P_y/P_x$	M	$V_x/V_y$	$T_y/T_x$
1-psi	1.068	1.02875	1.0481	1.01899
2	1.136	1.0567	1.0953	1.03716
3	1.204	1.084	1.1418	1.05473
4	1.272	1.1105	1.1870	1.07159
5	1.340	1.1364	1.2316	1.08801

where  $P_y/P_x$  is the pressure ratio (back to front) across a shock wave having a Mach number value of M and  $V_x/V_y$  is the velocity ratio (front to back) across the shock wave.

By definition,  $M = V_x/c_x$  and c is the speed of sound. For air,  $c = 49.02 \sqrt{T}$  where T is in °R and c is in feet-per-sec (ft/sec). Therefore, at 300 °F = 760 °R,  $c = 1351$  ft/sec.

The above values in Table 1 are for a coordinate system that is traveling with the shock wave, so that it is stationary relative to that coordinate system. For the purposes at hand, it is desirable to translate these values to a coordinate system wherein the gas that the shock wave is traveling into is stationary. That is, the gas in duct #86 and in Room 180 is stagnant.

The “high speed” setting for the Main Exhaust System fans is 300,000 cfm. The total cross-sectional area of the 17 ducts leading into the Plenum is 173.1 sq. ft. As a result, the average air speed to the filter bank in each duct is

$$300,000 \text{ ft}^3/\text{min} \times 1/173.1 \text{ ft}^2 = 1733 \text{ ft/min} \times (1 \text{ min}/60 \text{ sec}) = 28.9 \text{ ft/sec,}$$

and it will be shown below that this is small enough to be roughly neglected with respect to the airflow associated with the shock wave. Or, this value may be simply subtracted from the duct airflow speeds calculated below for the explosion.

To translate the moving coordinate system to one stationary with respect to Room 180 (the stagnant gas), the formula is

$$M_y' = c_x/c_y (M_x) - M_y \quad (10)$$

Now at a constant value of  $T_x = 300^\circ\text{F} = 760^\circ\text{R}$ , then  $c_x = 1351 \text{ ft/sec}$  is constant.

The  $M$  in Table 1 is  $M_x$ , and  $V_x$  is calculated using  $M_x$  and  $c_x$ . Then  $V_y$  is calculated using  $V_x/V_y$  and  $V_x$ . Also  $T_y$  is calculated using  $T_y/T_x$  and  $T_x$  so that  $c_y$  can be calculated from  $49.02\sqrt{T}$ . Finally,  $c_y$  and  $V_y$  are used to calculate  $M_y$ .

Table 2. Calculated Normal Shock Values for a Moving Coordinate System

Over-P	$T_y/T_x$	$T_y (^{\circ}\text{R})$	$c_y=49\sqrt{T}$	$V_x/V_y$	$V_x=M_x c_x$	$V_y$	$M_y=V_y/c_y$
1-psi	1.01899	774	1364	1.0481	1389	1325	0.971
2	1.03716	788	1376	1.0953	1428	1304	0.948
3	1.05473	802	1388	1.1418	1464	1282	0.924
4	1.07159	814	1399	1.1870	1500	1264	0.904
5	1.08801	827	1410	1.2316	1535	1246	0.884

Now equation (10) is used to calculate  $M_y' = V_y' / c_y$  since  $c_y' = c_y$ .

Table 3. Normal Shock Values for a Stationary Coordinate System

Overpressure	$M = M_x$	$M_y' = V_y' / c_y'$	$V_y' \text{ (ft/sec)}$	Flow in Duct #86 (mph)
1-psi	1.02875	0.0479	65.34	44
2	1.0567	0.0895	123.15	84
3	1.084	0.1311	181.97	124

Overpressure	$M = M_x$	$M_y' = V_y' / c_y'$	$V_y'$ (ft/sec)	Flow in Duct #86 (mph)
4	1.1105	0.1684	235.59	161
5	1.1364	0.2048	288.77	197

For the last column in Table 3, the flow-rate in duct #86 is calculated from  $V_y'$  (ft/sec) which is the flow-rate relative to the stationary duct, that is, as seen by a stationary observer in Room 180.

To convert flow speeds in feet-per-second (ft/sec) to miles-per-hour (mph) the following units conversion is used:

$$X \text{ ft/sec} \times (3600 \text{ sec} / 1 \text{ hr}) \times (1 \text{ mile} / 5280 \text{ ft}) \Rightarrow \text{miles per hour, or}$$

$$Y \text{ (mph)} = 0.6818 \times X \text{ (ft/sec)} \Rightarrow \text{Flow in \#86 duct in miles-per-hour.}$$

One intuitive way to look at gas flow is to follow chunks of mass flowing around the Plenum or ducts. The flow in the Plenum behind the moving shock wave is traveling at  $V_y'$  which indeed it is, since the blast pressure was calculated for the entire Plenum volume; i.e., enough CO (from both the filter media and lint/dust thrown into suspension by the “flame flashbacks”) was reacted in these calculations to heat the entire Plenum volume. Therefore, the blast wave is directly entering each duct at  $V_y'$  (or somewhat obliquely at approximately  $V_y'$ ).

It is realized that the foregoing is somewhat of a simplified view. There will, in fact, be three-dimensional flow patterns, such as the shock wave directly entering the ducts with some flow coefficient and the non-open area next to the ducts will reflect the wave and double its pressure in intensity. As a result, less pressure goes down the ductwork. However, mass does not disappear according the Law of Conservation of Mass, and indeed all the high-pressure (few psi) mass in the Plenum will flow out of the Plenum, although not exactly (but similarly) in the simplified one-dimensional manner as calculated here. Because of mass conservation, it is thought that following mass around will give a better feel for the flow and how it divides up into the downstream duct divisions.

The mass flowrate is given by  $m' = \tilde{n}VA$ , where  $\tilde{n}$  is the density,  $V$  is the

velocity and A is the cross-sectional area. Therefore, the mass flow into duct #86 is

$$m' \text{ (lb/sec)} = .07647 T_x/T_y \text{ (lb/ft}^3\text{)} \times V_y' \text{ (ft/sec)} \times 13 \text{ (ft}^2\text{)}$$

It was not quite clear from the original ventilation system schematic drawings if the flow into duct #86 divides into 7 or 9 separate exhaust ducts — discharge (flow) exits. However, there are at least 4 exhaust ducts in Room 180.

Note: The available 1957 revised floor plan drawing for Room 180 depicts 4 exhaust ducts in this room. However, only the original 1952 ventilation schematic drawings are available for review and no such exhaust ductwork is shown in the area occupied by the 1957 room layout.)

The effect of the Glovebox Booster Exhaust System ductwork will be disregarded since this flow path will only increase the flow into the Room 180 (i.e., the calculated results are conservative). As a conservative estimate for the massflow, the massflow will then be divided as 4/9. This is denoted as  $m'' = 4/9 m'$ . That is, the mass flowing into duct #86 will be proportioned so that 4 parts go into Room 180 and the other 5 parts of massflow will go to rooms other than Room 180 also serviced by this duct.

After the massflow in duct #86 ( $m'$ ) is divided into each of the 9 ducts, this massflow is then converted to volumetric flow  $VF''$  using the density of air ( $0.07647 T_x/T_y$  in lb/ft<sup>3</sup>). The speed through each grille at the exit of each of the 4 exhaust ducts in Room 180 can then be calculated noting that each grille is 3'-0"x1'-4" (as measured from the floor plan drawing); that is, the  $VF''$  in cubic-feet-per-second is divided by the flow area of 4-sq.ft and then multiplied by 0.6818 to convert ft/sec to mph denoted by  $SF''$  in Table 4.

Table 4. Massflow from Plenum Down Duct #86 into Room 180

Over-Press	$T_y$ (°R)	$V_y'$ (ft/sec)	$m'$ (lb/sec) Duct #86	$m''$ (lb/sec) each duct in Rm 180	$VF''$ (ft <sup>3</sup> /sec) each duct in Rm 180	SF'' (mph) each duct in Rm 180
1-psi	774	65.34	63.78	28.35	377.56	64
2	788	123.15	118.07	52.48	711.56	121
3	802	181.97	171.42	76.19	1051.4	179
4	814	235.59	218.66	97.18	1361.1	232
5	827	288.77	263.81	117.25	1668.4	284

## 2. Specific Thermodynamic Data And Conclusions

The gas-dynamic data calculated in Table 4 indicates the various shock wave speeds from the ducts entering Room 180 for various overpressures in the Plenum. Previously, the amount of carbon monoxide needed to generate a 10-psi overpressure was calculated to indicate that the generation of several psi was indeed consistent with the postulated phenomena. Now the amount of CO produced from the burning filter media and lint/dust thrown into suspension by the "flame flashbacks" needed to generate the overpressures of 1-3 psi in the Plenum will be calculated in order that a final comparison summary can be presented in Table 5 which will show that the numerical range for the variables is within the observed actual phenomena. This will then validate the postulated phenomena.

Starting with the calculation of equation (7) using  $P_i = 14.7$  and  $T_i = 760^\circ\text{R}$  then  $T_f = P_f/P_i \times N_f/N_i \times T_i$ . Then the values of  $T_f$  (°R) are used to look up the tabulated values for internal energy in Btu/lb. The value of  $u_{\text{air}}$  at the initial  $300^\circ\text{F}$  ( $u_{\text{air}} = 129.99$  Btu/lb) is then subtracted to get  $\Delta u$ . The required Btu to heat the Plenum to get the  $\Delta u$  is then calculated by multiplying by the Plenum mass of  $5110 \text{ lb}_{\text{air}}$ . The Btu needed is then divided by the heat given off by CO reaction per pound of CO =  $4342 \text{ Btu/lb}_{\text{CO}}$ . The number of clean and dirty filters required to be consumed to generate sufficient CO to cause the explosion are then calculated. The last column of data in Table 5 shows the amount of dirty filters needed to generate sufficient CO to

cause the explosion if only one-third of the cellulosic mass of the dirty filters was consumed by smoldering. Although the filters in the plenum were dirty, the data in Table 5 for clean filters was computed as "limit" calculation.

Table 5. Number of Filters Needed to be Burned to Provide the Overpressure

P	T <sub>f</sub> (°R)	u <sub>air</sub>	Äu	Btu	lb <sub>CO</sub>	Clean	Dirty*	1/3-Dirty**
1-psi	953.9	164.17	34.18	176,335	40.6	2.4	1.5	4.5
2	1013.3	174.83	44.84	231,330	53.3	3.1	2.0	5.9
3	1074.0	185.99	56.00	288,904	66.5	3.9	2.4	7.3
4	1134.6	196.94	66.95	345,395	79.5	4.6	2.9	8.8
5	1195.3	208.48	78.49	404,930	93.3	5.4	3.4	10.3

\*Dirty involves a filter loaded with lint and associated dust (17.2 lbs. cellulose filter media plus 10 lbs. cellulose lint/dust equals 27.2lbs. cellulose).

\*\*1/3 Dirty (27.2 lbs. ÷ 3 = 9.07 lbs. cellulose).

Using Table 4 and interpolating the data, and stating that it takes approximately 100-mph to knock a person down, then an overpressure of 1.6 psi in the Plenum would be sufficient in the "ideal no-pressure loss" approximation. However, at this time, some realistic losses in the system will be considered. Duct #86 starts out of the Plenum at 13 ft<sup>2</sup>. It then has two 90°-bends before branching to an 11.56 ft<sup>2</sup> duct for the main-run. This 11.56 ft<sup>2</sup> main-duct then reduces down to a 9.4 ft<sup>2</sup> main-run and then to a 6.5 ft<sup>2</sup> main-run which terminates in Room 180. Two branches of 10.5 ft<sup>2</sup> come off the 11.5 ft<sup>2</sup> main-run duct, then two branches of 8.7 ft<sup>2</sup> come off the 9.4 ft<sup>2</sup> main-run, and, finally, two branches of 5.4 ft<sup>2</sup> come off the 6.5 ft<sup>2</sup> main-run duct and extend to other rooms/areas served by duct #86. None of these ducts are small, and the existing balancing dampers are not considered to cause a significant pressure loss. Therefore, a realistic pressure loss through the duct is in the order of 1 psi. To obtain a flow of 100 mph in Room 180, it might realistically require an overpressure of 2.6 psi in the Plenum instead of the "ideal" amount of 1.6 psi predicted in Table 4. This 2.6 psi buildup is what would have originally existed in the plenum due to the explosive burning of CO from the smoldering of the cellulosic filter media and suspended lint/dust in the upstream ("dirty air") side of the plenum. As this overpressure expended, it pushed air and products of combustion

(containing plutonium) into the ductwork and produced a flow of 100 mph.

In summary, it is known that the explosion in the Plenum caused a 1 psi overpressure upstream in Room 180, which was sufficient to knock personnel down. Likewise, the lack of structural damage to the Plenum indicates that the pressure generated by the explosion within the Plenum was below 2.6 psi overpressure.

**D. Physical Effects and How They Relate to the Calculations**

A discussion is now presented about the physical effects and the time and temperature factors that support the blast scenario and the succeeding calculations.

The Critical Time-Line for the events is as follows:

10:10 p.m.	Fire discovered
10:25 p.m.	Fans for main exhaust system placed on high speed (300,000 cfm)
10:28 p.m.	Smoke noticed coming from exhaust system stack
10:37 p.m.	Water spray directed at fire
10:38 p.m.	Fire extinguished
10:39 p.m.	Explosion in exhaust system per fire report
10:39+p.m.	Re-ignition of fire in Room 180
10:40 p.m.	Main exhaust fans went off

The only plausible time-sequence scenario for the above time-line events is as follows:

- a. Fire initiation in Room 180.
- b. Booster filters burn through due to their close proximity to the heat generated from the fire in Room 180 and cause burn-through of several filters in the Plenum. Due to the relatively large/heavy particulate from the Booster filters, the Plenum filters that failed due to the failure of the Booster filters were those downstream of and directly across from Duct #86 since the particulate may not have followed the airflow direction in the Plenum and therefore tend to flow in a straight direction.
- c. Heat from the fire in Room 180 continues through the Booster duct and airflow ducts to heat the Plenum filters and raise their temperature.
- d. Smoldering of the Plenum filters continues until a critical temperature is

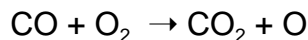


reached whereby a critical concentration of carbon monoxide [CO] is reached.

- e. Carbon monoxide reacts with the oxygen and other chemical species (e.g., OH) to release a large amount of chemically-generated energy, resulting in a rapid pressure increase in the Plenum.

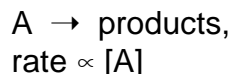
Now the details of how such phenomena can occur is presented. First, in the extreme case, let us assume that all the carbon monoxide from the Booster filters and the few/several Plenum filters that failed has been swept away by the airflow due to the main exhaust fans. But it is known that the fire in Room 180 is continuing and the resultant heat is being drafted through the duct-work to the Plenum so that the Plenum filters are being heated so their temperature is increasing.

The phenomenological law of mass action, which is confirmed experimentally, states that the rate of a reaction is proportional to the product of the concentrations of the reactants. For a reaction such as



the rate at which the above reaction proceeds to the right to form  $\text{CO}_2$  is proportional to the concentrations of the chemical species (CO and  $\text{O}_2$ ) on the left side of the arrow.

In simple terms, for the elementary reaction



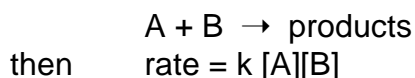
where [A] denotes the concentration of species A, and

$$\text{rate} = k[\text{A}]$$

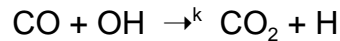
where k is a coefficient known as the rate coefficient.

The value of this coefficient will depend on the nature of the reaction (i.e., the type of species involved) and will normally vary with the temperature, but is not a function of concentration.

If the chemical reaction is such that more than one molecule is concerned in the process, for example



For the reaction

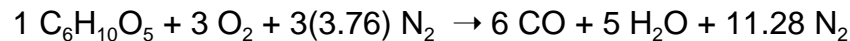


the rate of formation of  $\text{CO}_2$  is given by

$$d[\text{CO}_2]/dt = k [\text{CO}] [\text{OH}]$$

where the square brackets [ ] indicate concentration of a species and k is the proportionality constant which is called the reaction rate coefficient for that specific elementary reaction. The left side of the equation,  $d[ ]/dt$ , gives the rate of formation of carbon dioxide.

The reaction



is not an elementary reaction but a representation of the overall process and is called an overall reaction as differentiated from an elementary reaction which represents the actual species (molecules) that collide and react.

Almost without exception, a rise in temperature produces an increase in the rate of reaction. The statement that “a rise in temperature of 10°C may double the rate” gives an approximate idea of such an increase; the factor is commonly between 1 and 3. Thus for a rise of 100°C, a thousand fold increase in rate is not unexpected. The usual observed increase in rate of reaction is due essentially to an increased efficiency of collisions which lead to reaction, in the sense that only such molecules which have energy equal to or greater than a certain critical value (the energy of activation) can react. The fraction of molecules which are so activated is given by the Boltzmann factor  $e^{-E/RT}$  where E is the energy of activation., R the gas constant and T the absolute temperature. The form of this factor is such that its value will increase rapidly with rise in temperature (the form is exponential) and the rise in chemical reaction rate is in fact largely due to this cause.<sup>(25h)</sup>

Temperature is an indication of the energy. As energy from heat transfer is added, then the temperature is increased and the molecules are more energetic. As heat is added at the upstream interface of a mass of gas or solid, the energy is transferred very rapidly to the neighboring molecules by molecular collisions. Chemical reaction thus takes place when the molecules are raised to a sufficiently high energy state, usually by collision. The molecules are then said to be activated or to form an activated complex, of an energy higher by E than the normal un-activated molecules.

For the reaction  $\text{A} + \text{B} \rightarrow \text{products}$  with rate =  $k [\text{A}][\text{B}]$

the quantitative relationship between the rate coefficient, k, and temperature is of the form  $k = A e^{-E/RT}$  where A and E are taken to be constant for a given reaction over the temperature range concerned. The rate coefficient, k, is then considered to be

made up of two rate factors: the Boltzmann factor  $e^{-E/RT}$  to which the change with temperature is due, and the A factor which is referred to as the 'frequency factor'. The frequency factor, A, is indicative of: (1) the types of molecules involved (the types and configurations of the atoms); (2) the way in which vibrational energy is distributed and; (3) the orientation of the colliding molecules. In simple terms for chemical reaction, two molecules react when they collide with sufficient energy (activation energy, E), and **the reaction rate coefficient increases exponentially as the temperature increases linearly.**

With respect to cellulose fiber and lint/dust for the case at hand, the cellulose is being heated by the hot gases from the fire in Room 180. In the early stages, the decomposition of the cellulose due to its smoldering caused by heating is relatively slow and products such as decomposed cellulose species and carbon monoxide are swept away by the airflow caused by the exhaust fans and buoyancy due to the heat. It is noted that this 'sweeping away' is a linear process and is relatively very slow as compared to the generation of CO in the later stages of smoldering (i.e., chemical reaction). The upstream cross-sectional area of the Plenum is 3,373 square-feet (230-feet wide x 14-feet+8-inches high) and the airflow (when fans on high) is 300,000 CFM. Dividing 300,000 by 3373 gives a linear flow rate of 88.9 feet-per-minute or 1.48 feet-per-second; therefore, it would take several seconds for this flow to move the 9.5-feet depth of this Plenum. As the filter media continues to be heated and the temperature increases, the reaction rate is **increasing exponentially**. When enough heat is transferred to the cellulosic filter media and cellulosic lint, and oxygen is being supplied by the forced convection of the exhaust fans (now on high speed), the temperature of the smoldering process increases to the point where the **exponential** formation of CO outweighs the loss of CO due to the **linear** forced airflow, and a very fast chemical reaction of CO to CO<sub>2</sub> occurs (on the order of milliseconds). This results in releasing a large amount of energy which very rapidly expands the hot gases and creates a pressure wave.

To substantiate the above comments, the following information obtained from the SFPE Handbook<sup>(27b)</sup> is provided:

Note:     Italicized comments in parenthesis are provided by the Report Writer.  
              Highlighted information is for emphasis.

- a. "Smoldering is a slow, low-temperature, flameless form of combustion, sustained by the heat evolved when oxygen directly attacks the surface of a condensed-phase fuel. ... Smoldering provides a pathway to flaming that can be initiated by heat sources much too weak to directly produce a flame."

*(Note: It should be noted that smoldering filter media in clean or plugged filters and lint could occur within the Plenum with the exhaust fans operating at high speed and producing ten air changes per minute.)*

- b. “A burning cigarette is a familiar example of this flameless mode of combustion (Note: the cigarette phenomenon is similar to cellulosic filter media and lint) and has several characteristics common to most materials that smolder.” The leading surface of “finely divided fuel particles (i.e., tobacco) provide large surface area per unit mass of fuel, which facilitates the surface attack by oxygen. ... The permeable nature of the aggregate of fuel particles permits oxygen transport to the reaction site by diffusion and convection. ... At the same time, **such particle aggregates typically form fairly effective thermal insulators that help slow heat losses, permitting sustained combustion despite low heat release rates.**” *(Note: It is for these reasons that lint within the inlet side of the Plenum could continue to smolder and generate CO even with high airflow.)*
- c. “The physical factors that favor smoldering must be complemented by chemical factors as well. Like virtually all other cellulosic materials, tobacco in a cigarette, when degraded thermally, forms a char. A char is not a well-defined material, but typically it is considerably richer in carbon content than the original fuel; its surface area per unit mass is also enhanced. This char has a rather high heat of oxidation and is susceptible to rapid oxygen attack at moderate temperatures ( $\geq 397^{\circ}\text{C}$ ).” (Table 1-23.1 shows that the maximum temperature for smoldering of cellulose fabric is  $770^{\circ}\text{C}$ ) “The attack of oxygen (**to form mainly carbon monoxide** and carbon dioxide) is facilitated not only by the enhanced surface area but also by alkali metal impurities (present in virtually all cellulosic materials derived from plants) which catalyze the oxidation process.” *(Note: It is for this additional reason that lint would continue to smolder and generate CO within the Plenum even with the large airflow produced by the fans on high speed.)*
- d. “The smolder initiation process is dominated by the kinetics of the oxidation of the solid. Subsequent propagation of smolder is controlled to a large degree, however, by the rate of oxygen transport to the reaction zone. The control via transport rate occurs because **the heat evolved during smolder initiation raises the local temperature and thus the local reaction rate.**” *(Note: It should be noted that as the heat from Room 180 raises the temperature of the filter media and lint, the smoldering reaction rate within the Plenum is increasing.)*

- e. “A well-insulated reaction zone is a key factor in the existence of stable, self-sustaining smolder at such extremely low rates. The heat loss rate cannot exceed the heat generation rate. In this case, the same factor that is slowing the oxygen supply rate, and therefore the heat generation rate” (i.e., the thick layer of cellulosic filter media and lint particles over the reaction zone which is internal to the filter media and lint particles) “is also slowing the heat loss rate. ... The smolder propagation process is inherently unsteady because of the time-dependent oxygen supply process. If oxygen is instead continually supplied by a forced convective flow through the fuel layer, nearly steady propagation occurs.” *(Note: It should be noted that as high-speed fan operation produces increased ventilation of the Plenum area and oxygen flow through the burning filters, continued generation of CO occurs.)*
- f. “Thermal degradation of some fuels in the presence of oxygen is exothermic. This is particularly true of cellulosic materials (e.g., filter media and lint) and this heat can be sufficient to drive the smolder wave without any char oxidation.” *(Note: In the filter Plenum fire, the smoldering of the filter media and lint releases heat [exothermic] which raises the local temperature to allow the smoldering process and generation of CO to escalate — even with the large airflow in the Plenum.)*
- g. “The participation of oxidative/thermal degradation in driving the smolder process requires that oxygen have free access to the thermal degradation region. For a low-permeability fuel such as solid wood, this is not the case. Even though solid wood has basically the same reaction chemistry as cellulosic insulation (which consists mostly of wood fibers) and smolders with a qualitatively similar inclined reaction zone, it must be driven solely by char oxidation. The low permeability and corresponding high density of solid wood has another consequence with regard to smolder. The self-sustaining quality of the reaction zone is much less than with a low-density layer of fuel particles or fibers.” *(Note: It is therefore concluded that, although the wood filter-frames may have burned to some degree, the higher permeability of the filter media and lint would lead to higher formation rates for CO than wood at the same heat input because of the lower permeability of the solid-wood filter-frames.)*
- h. “Transition to flaming (fast exothermic gas-phase reactions) requires both a mixture of gases and air that are within their flammability limits, and a sufficient heat source to ignite this mixture. Furthermore, these two

requirements must be realized at the same locus in space and at the same time. Any factor that either enhances the net rate of heat generation or decreases the net rate of heat loss will move the smoldering material toward flaming ignition by increasing both local temperature and rate of pyrolysis gas generation. Such factors include an enhanced oxygen supply....”

*(Note: The accumulated lint on the surface of the filter media will react similarly to the filter media because both are cellulosic material. However, lint may lead to significant reaction beyond smoldering at a different temperature, because its physical configuration is different from the cellulosic filter media, resulting in differences for physical and chemical processes. It seems likely that the accumulated lint itself, in combination with the filter media, led to the pressure pulse which then may have dislodged material. Therefore, after the exhaust fans were placed on high speed, the accumulated lint, which remained on the outer surface of the filter media, smoldered and contributed (along with the filter media) to produce sufficient quantities/rates of CO to achieve the Lower Explosive Limit (LEL) locally within the Plenum. At the time of the explosion, it is theorized that unburned lint, that was dislodged from the filters through vibrations exerted on the filter bank through the numerous flashbacks, would have reacted simultaneously during the rapid chemical reaction of CO initiated through ignition via flames from one of the numerous flashbacks, regardless of the large airflow occurring in the Plenum area. This would have occurred since lint in suspension presents a finely divided media (i.e., dust), that reacts extremely rapidly because heat transfer is inversely proportional to the square of the diameter. For example, if the diameter of a fiber of suspended lint is one-fourth that of the filter media then the heat transfer rate is increased by a factor of sixteen. The increase in heat transfer rate then increases the temperature proportionately ( $Q \propto \Delta T$ ) and increases the reaction rate exponentially (that is why dust explosions occur readily). The calculated weight of cellulosic material for clean and dirty (with lint) filters needed to achieve the lower explosive concentration of CO are presented in Table 5 of this Section. In the case at hand, eventually enough of the filter media and lint has pyrolyzed to produce a sufficient amount of combustibles in the lower explosive limit range so that reaction of these accumulated species leads to a rapid heat release rate from chemical reactions. These reactions then cause a rapid expansion of the surrounding gases that results in a pressure wave).*

- i. “A further factor in this and in other systems involving cellulosic materials is secondary char oxidation. This process is quite similar to the afterglow

seen in cellulosic chars left by flaming combustion. Intense, high-temperature (probably greater than 1070 K) reaction fronts propagate intermittently in seemingly random directions through the fibrous low-density char left by the main lower temperature smolder front. In charred fabrics, these glowing fronts can sometimes progress in a stable manner along the charred residue of a single fiber, despite very high heat losses per unit volume of fuel.” *(Note: Although it may appear at first glance that heat is lost rapidly to airflow, it has been demonstrated that the charred residue of a single fiber, such as lint for the case at hand, forms a char complex internally that prevents rapid loss of heat so that chemical reaction does indeed occur in spite of the large air flow.)*

- j. “The transition from smolder to flaming can also be induced, for example, by a forced increase in oxygen supply rate to the smolder reaction zone.” “These heat transfer effects intensify the smolder in the leading edge region for forward smolder. In the case of cellulosic insulation, the intensification leads to random development of small (a few cm) cavities near the leading edge which act as flame initiation regions and flame holders.” *(Note: When the main exhaust fans were turned onto high speed, this forced increase in oxygen supply rate to the smolder reaction zone led to very high energy release rates from chemical reaction.)*

From the above discussion it is concluded that heat from the fire in Room 180 and the early heat and burning embers from the Booster exhaust system filters caused the initial smoldering of the cellulosic filter media and lint in the Plenum, and that the rising temperature led to the exponential increase in reaction rates until a critical concentration of CO accumulated. This critical concentration of CO, known as the LEL, produced in spite of the large airflow within the Plenum, then reacted explosively along with the lint that was vibrated into suspension to generate a blast pressure wave in the Plenum which resulted in knocking down personnel in Room 180.

\*\*\* END OF SECTION IV \*\*\*